Electronic structure of magnetically modulated graphene

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(Date textdate; Received date; Revised date; Accepted date; Published date)

Abstract

We present a theoretical study of the electronic structure of magnetically modulated graphene. We consider monolayer graphene in the presence of a perpendicular magnetic field and a unidirectional weak magnetic modulation. The density of states and the bandwidth of the Dirac electrons in this system are determined. We have found magnetic Weiss oscillations in the bandwidth and the density of states. These oscillations are out of phase and larger in amplitude than the ones in the electrically modulated graphene. In addition, these oscillations are in phase and smaller in amplitude to those of magnetically modulated standard electron gas system.

I. INTRODUCTION

The successful preparation of monolayer graphene has allowed the possibility of studying the properties of electrons in this system[1]. The nature of quasiparticles called Dirac electrons in these two-dimensional systems is very different from those of the conventional two-dimensional electron gas (2DEG) systems realized in semiconductor heterostructures. Graphene has a honeycomb lattice of carbon atoms. The quasiparticles in graphene have a band structure in which electron and hole bands touch at two points in the Brillouin zone. At these Dirac points the quasiparticles obey the massless Dirac equation. In other words, they behave as massless Dirac particles leading to a linear dispersion relation $\epsilon_k = vk$ (with the characteristic velocity $v \simeq 10^6 m/s$). This difference in the nature of the quasiparticles in graphene from conventional 2DEG has given rise to a host of new and unusual phenomena such as anomalous quantum Hall effects and a π Berry phase[1, 2, 3]. Besides the fundamental interest in understanding the electronic properties of graphene there is also serious suggestions that it can serve as the building block for nanoelectronic devices [4]. Since Dirac electrons can not be confined by electrostatic potentials due to the Klein's paradox it was suggested that magnetic confinement be considered [5]. Technology for this already exists as the required magnetic field can be created by having ferromagnetic or superconducting layers beneath the substrate [6].

In conventional 2DEG systems, electron transport in the presence of electric[7, 8, 9] and magnetic modulation[10, 11, 12] has continued to be an active area of research. In graphene, electrical transport, density of states, bandwidth, thermodynamic properties and collective excitations in the presence of electrical modulation have been considered and theoretical predictions made [13, 14, 15]. It is interesting to study the affects of the magnetic modulation on the Dirac electrons in a graphene monolayer and investigation in this direction has recently been carried out [16, 17]. In this work we study the effects of magnetic modulation on the bandwidth (Δ) and the density of states (DOS) of the Dirac electrons in graphene. Both these quantities are essential ingredients in studying problems such as electron transport, collective excitations and thermodynamic properties etc. We consider an external magnetic field perpendicular to the graphene monolayer that is modulated weakly and periodically along one direction. We find that the magnetic Weiss oscillations in the bandwidth and density of states are out of phase and larger in amplitude than the electric Weiss oscillations

found in the corresponding electrically modulated system.

In section II, we present the formulation of the problem. Section III contains the calculation of the density of states. Bandwidth for magnetically modulated graphene is discussed in section IV followed by conclusions in section V.

II. FORMULATION

We consider two-dimensional Dirac electrons in graphene moving in the x-y-plane. The magnetic field (B) is applied along the z-direction perpendicular to the graphene plane. The perpendicular magnetic field B is modulated weakly and periodically along one direction such that $\mathbf{B} = (B + B_0 \cos(Kx))\widehat{z}$. Here B_0 is the strength of the magnetic modulation. In this work we consider the modulation to be weak such that $B_0 << B$. We consider the graphene layer within the single electron approximation. The low energy excitations are described by the two-dimensional (2D) Dirac like Hamiltonian ($\hbar = c = 1$ here) [1, 2, 16]

$$H = v\overleftrightarrow{\sigma}.(-i\nabla + e\overrightarrow{A}). \tag{1}$$

Here $\overleftrightarrow{\sigma} = \{\overleftrightarrow{\sigma}_x, \overleftrightarrow{\sigma}_y\}$ are the Pauli matrices and v characterizes the electron velocity. We employ the Landau gauge and write the vector potential as $\overrightarrow{A} = (0, Bx + (B_0/K)\sin(Kx), 0)$ where $K = 2\pi/a$ and a is the period of the modulation. The Hamiltonian given by Eq. (1) can be expressed as

$$H = -iv\overleftrightarrow{\sigma}.\nabla + ev\overleftrightarrow{\sigma_y}Bx + ev\overleftrightarrow{\sigma_y}\frac{B_0}{K}\sin(Kx).$$

The above Hamiltonian can be written as

$$H = H_0 + V'(x) \tag{2}$$

where H_0 is the unmodulated Hamiltonian and V' is the perturbation potential due to the periodic magnetic field in one direction such that

$$H_0 = -iv\overleftrightarrow{\sigma}.\nabla + ev\overleftrightarrow{\sigma_y}Bx$$

and

$$V'(x) = \omega_0\overleftrightarrow{\sigma_y}\sin(Kx).$$

where $\omega_0 = \frac{evB_0}{K}$. The Landau level energy eigenvalues without modulation are given by

$$\varepsilon(n) = \omega_g \sqrt{n} \tag{3}$$

where n is an integer and $\omega_g = v\sqrt{2eB}$. As has been pointed out [13, 16] the Landau level spectrum for Dirac electrons is significantly different from the spectrum for electrons in conventional 2DEG which is given as $\varepsilon(n) = \omega_c(n + 1/2)$, where $\omega_c = eB/m$ is the cyclotron frequency.

The eigenfunctions without modulation are given by

$$\Psi_{n,k_y}(r) = \frac{e^{ik_y y}}{\sqrt{2L_y}} \begin{pmatrix} -i\Phi_{n-1}(x, x_0) \\ \Phi_n(x, x_0) \end{pmatrix} \tag{4}$$

where

$$\Phi_n(x, x_0) = \frac{e^{-(x-x_0)^2/2l}}{\sqrt{2^n n! \sqrt{\pi} l}} H_n(\frac{x - x_0}{l})$$

where $l = \sqrt{1/eB}$ is the magnetic length, $x_0 = l^2 k_y$, L_y is the y-dimension of the graphene layer and $H_n(x)$ are the Hermite polynomials. Since we are considering weak modulation $B_0 << B$, we can apply standard perturbation theory to determine the first order corrections to the unmodulated energy eigenvalues in the presence of modulation

$$\Delta\varepsilon_{n,k_y} = \int_{-\infty}^{\infty} dx \int_0^{L_y} dy \Psi^*_{n,k_y}(r) H'(x) \Psi_{n,k_y}(r) \tag{5}$$

with the result

$$\Delta\varepsilon_{n,k_y} = \omega_0 \cos(Kx_0) \left(\frac{2\sqrt{n} e^{-u/2}}{Kl} [L_{n-1}(u) - L_n(u)] \right) \tag{6}$$

where $u = K^2 l^2/2$ and $L_n(u)$ are the Laguerre polynomials. Hence the energy eigenvalues in the presence of modulation are

$$\varepsilon(n, k_y) = \varepsilon(n) + \Delta\varepsilon_{n,k_y} = \omega_g \sqrt{n} + \omega_0 G_n(u) \cos(Kx_0) \tag{7}$$

with $G_n(u) = \frac{2\sqrt{n}}{Kl} e^{-u/2}[L_{n-1}(u) - L_n(u)]$. We observe that the degeneracy of the Landau level spectrum of the unmodulated system with respect to k_y is lifted in the presence of modulation with the explicit presence of k_y in x_0. The $n = 0$ Landau level is different from the rest of the levels as the energy of this level vanishes and no modulation induced broadening of this level occurs. The rest of the Landau levels broaden into bands. The

Landau bandwidths $\sim G_n$ oscillate as a function of n since $L_n(u)$ are oscillatory functions of the index n.

Before we begin the calculation of the density of states and the bandwidth, it is necessary to discuss the regime of validity of the perturbation theory presented here. For large n the level spacing given by Eq. (3) goes as $\omega_g(\sqrt{n} - \sqrt{(n-1)}) \longrightarrow \omega_g \frac{1}{2\sqrt{n}}$ and the width of the nth level given by Eq.(6) goes as $\frac{2\omega_0 n^{1/2}}{Kl}$. There is therefore a value of n at which the width becomes equal to the spacing and the perturbation theory is no longer valid. This occurs when $n_{\max} = \sqrt{2}\pi^2 \frac{B'}{B_0}$ where $B' = \frac{1}{ea^2} = 0.0054T$ for a fixed value of $a = 350nm$. For a fixed electron density and the period of modulation this suggests the maximum value of the magnetic modulation B_0 above which it is necessary to carry out a more sophisticated analysis.

At this stage we can compare the energy spectrum of Dirac electrons in magnetically modulated graphene with both the electrically modulated graphene system and the electrically modulated standard electron system. The differences are:

• The standard electron unperturbed energy eigenvalues depend linearly on the magnetic field and the quantum number n while they depend on the square root of both the magnetic field and n for the Dirac electrons in graphene.

• In magnetically modulated graphene, we have the difference of two successive Laguerre polynomials while for standard electrons and electrically modulated graphene, we have the sum and average of the two successive Laguerre polynomials respectively.

• In magnetically modulated graphene the perturbed energy eigenvalues due to modulation are multiplied by the square root of the Landau band index $\sqrt{n}$ that was absent in the expression for the electric case.

These differences will affect the density of states and the band width as we show in the next section. Note that for a weak magnetic modulation case under consideration the quantum numbers n can be referred to as the magnetic Landau band indices and are equivalent to the Landau level quantum number n for the unmodulated system. Thus the magnetic modulation induced broadening of energy spectrum is non-uniform, a feature which will be of significance in understanding the behavior of Dirac electrons in modulated graphene.

III. THE DENSITY OF STATES (DOS)

It is well known that in the absence of both the magnetic field and modulation, the DOS consists of a series of delta functions at energies equal to $\varepsilon(n)$. The addition of a weak spatially periodic magnetic modulation however modifies the former delta function like DOS by broadening the singularities at the energies($\varepsilon(n)$) into bands. The density of states is given by

$$D(\varepsilon) = \frac{1}{A}\sum_{nk_y}\delta(\varepsilon - \varepsilon(n, k_y)). \tag{8}$$

The sum on n extends over all occupied Landau levels and A is area of the sample. By using the energy eigenvalues given in equation (7), we can express $D(\varepsilon)$ as:

$$D(\varepsilon) = 2\frac{1}{2\pi a l^2}\sum_{n}\int_{0}^{a} dx_0 \delta(\varepsilon - \varepsilon_n - |G_n|\cos(Kx_0)), \tag{9}$$

where $\varepsilon_n = \omega_g\sqrt{n}$, and a factor 2 is due to spin degeneracy. Evaluation of the x_0-integral in the above equation yields the zero temperature density of states of the density modulated two-dimensional Dirac electrons (DM2DDE):

$$D(\varepsilon) = \frac{1}{\pi^2 l^2}\sum_{n}\frac{1}{\sqrt{|G_n|^2 - (\varepsilon - \varepsilon_n)^2}}\theta(|G_n| - |\varepsilon - \varepsilon_n|). \tag{10}$$

where $\theta(x)$ is the Heaviside unit step function. Here we can see that the one-dimensional van Hove singularities of the inverse square-root type exist on either side of the low and high energy edges of the broadened Landau bands forming a double peak like structure.

The dimensionless density of state as a function of energy at $B = 0.35T$ is shown graphically in Fig.(1) as a function of $1/B$, for both the magnetically and electrically modulated graphene using the following parameters [13, 14, 15, 16]: $v \simeq 10^6 m/s$, $n_D = 3 \times 10^{15}$ m^{-2}, $a = 350$nm, $\omega_0 = 1$ meV, and $k_F = (2\pi n_D)^{1/2}$ being the Fermi wave number of the unmodulated system in the absence of magnetic field. The modulation induced pronounced oscillations are apparent in the weak magnetic field regime, these are the Weiss oscillations, superimposed on SdH-type oscillations in the high field regime that are not induced in our results but it is interesting to highlight their characteristics. The origin of these two types of oscillations can be understood by a closer analytic examination of equation (10). In the regime $\omega_g > |G_n|$, the unit step function vanishes for all but the highest occupied Landau band corresponding, say, to the band index N. Hence the sum over n is trivial. The

analytic structure primarily responsible for the Weiss type of oscillations is the function $\theta(|G_n| - |\varepsilon - \varepsilon_n|)$, which jumps periodically from zero (when the Fermi level is above the highest occupied Landau band) to unity (when the Fermi level is contained with in the highest occupied Landau band), these oscillations are with constant period in $1/B$ similar to the SdH type of oscillations in case of electrically modulated graphene but are out of phase and larger in amplitude. On the other hand, modulation of the amplitude of the Weiss oscillations displayed in Fig. (1) is largely a consequence of the oscillatory factor G_N, which exhibits commensurability oscillations. We also find that the minima of the density of states in the magnetically modulated system occur at the maxima of the electrically modulated one with the result that the oscillations in the density of states in the two systems are out of phase. We also observe that broadening of the Landau levels is greater in magnetically modulated graphene compared to electrically modulated graphene. In addition, van Hove singularities forming double peak like structures appear at the low and high energy edges of the broadened Landau levels.

IV. THE BANDWIDTH (Δ)

To better appreciate the modulation of the amplitude of Weiss oscillations we plot the bandwidth as a function of the magnetic field in Fig. 3. The width of the nth Landau level is given as

$$\Delta = 2\,|G_n| = \frac{4\omega_0\sqrt{n}}{Kl}e^{-u/2}[L_{n-1}(u) - L_n(u)] \tag{11}$$

This is clearly different from the electrically modulated graphene and magnetically modulated standard electron result [10, 11, 12]. The bandwidth is plotted for $n = n_F$ where $n_F = E_F^2/\omega_g^2$ is the Landau level index at the Fermi energy similar to the electrically modulated graphene system[to compare $n_F = \frac{E_F}{\omega_c} - \frac{1}{2}$,with $\omega_c = \frac{eB}{m}$ for standard electrons in 2DEG]. In Fig.(2) we present the bandwidths as a function of the magnetic field for both the magnetically modulated graphene and electrically modulated graphene. The parameters used in the figures are: $v \simeq 10^6 m/s$, $n_D = 3 \times 10^{15}$ m^{-2}, $a = 350$nm, $\omega_0 = 1$ meV, and $k_F = (2\pi n_D)^{1/2}$. The bandwidths as a function of the magnetic field for the magnetically modulated graphene and magnetically modulated 2DEG are shown in Fig.(3). For the low magnetic fields under consideration, the magnetic modulation induced bandwidth in graphene is out of phase and larger in amplitude (~ 1.5 times larger at magnetic field

$B = 1T$) than the electric modulation induced bandwidth in graphene. In addition, it is in phase but with smaller amplitude (~ 5 times smaller at magnetic field $B = 1T$) compared to the magnetically modulate 2DEG system.[10, 11, 12]. An analysis of the observed change in amplitude of the oscillations in the bandwidths of the three systems considered here is presented in the next section.

A. Asymptotic Expression

The asymptotic expression of bandwidth can be obtained by using the folowing asymptotic expression for the Laguerre polynomials in the limit of large n as

$$exp^{-u/2} L_n(u) \rightarrow \frac{1}{\sqrt{\pi\sqrt{nu}}} \cos(2\sqrt{nu} - \frac{\pi}{4}) \tag{12}$$

Using $n = n_F = E_F^2/\omega_g^2$ and substituting the asymptotic expression given by equation (12) into equation (11) yields the asymptotic expression for the bandwidth

$$\Delta = \frac{8\omega_0\sqrt{n_F}}{Kl} \frac{1}{\sqrt{\pi\sqrt{n_F u}}} \sin\left(1/2\sqrt{u/n_F}\right) \sin\left(2\sqrt{n_F u} - \frac{\pi}{4}\right),$$

$$\Delta = \frac{8\omega_0}{Kl} \frac{1}{\sqrt{\frac{\pi^2 R_g}{a n_F}}} \sin\left(\frac{\pi R_g}{2an_F}\right) \sin\left(\frac{2\pi R_g}{a} - \frac{\pi}{4}\right), \tag{13}$$

where we have rewritten equation (11) containing $u = K^2l^2/2$ in terms of the ratio of the semi-classical orbital radius R_g and the modulation period a.

To better understand the increase in amplitude in the magnetically modulated graphene system compared to the electrically modulated one we consider the difference in bandwidths in the two cases [13, 15]. Important feature is the additional $\sin\left(\frac{\pi R_g}{2an_F}\right)$ term and a factor of $\sqrt{n}$ in the perturbed energy eigenvalues for the magnetically modulated case which is absent in the electrically modulated case. For large value of n, $\sin\left(\frac{\pi R_g}{2an_F}\right)$ can be taken to be equal to $\frac{\pi R_g}{2an_F}$ and the amplitude of the oscillations in the bandwidth of the magnetically modulated graphene becomes smaller due to this factor compared to the magnetically modulated 2DEG. The result is that the bandwidth in the magnetically modulated $\left(\frac{2\sqrt{n}}{Kl}\sqrt{\frac{u}{n}} \approx 1.5\right)$ case is approximately greater by a factor of 1.5 compared to the electrically modulated $\left(\frac{a}{\pi^2 l\sqrt{\frac{K_F}{2eB}}} = 0.87\right)$ graphene system at magnetic field strength B=1 Tesla and it is smaller by a factor of 5 compared to the magnetically modulated ($\frac{aK_F}{2\pi} = 7.6$) standard electron gas.

B. Classical description

We now give a classical explanation of the asymptotic expression of bandwidth obtained in equation (13) which is essentially a large n expression. The classical equations of motion along the x and y directions are $x(t) = x_0 + R_g sin(\omega_g t + \varphi)$ and $y(t) = y_0 + R_g cos(\omega_g t + \varphi)$, respectively, where $\omega_g = v\sqrt{2eB}$, is the cyclotron frequency for Dirac electrons, R_g is the cyclotron orbit radius in graphene while x_0 and y_0 are the center coordinates and φ is the phase factor. Note that $\omega_c = \frac{eB}{m}$ for standard electrons which is not the same as what we have for Dirac electrons given above. Now without loss of generality we may take $\varphi = 0$. Thus the increase in the average energy of the cyclotron motion due to the magnetic modulation is evaluated as

$$\Delta E(x_0) = \frac{1}{t_0} \int_{-\frac{t_0}{2}}^{+\frac{t_0}{2}} \omega_0 \sin(Kx(t))dt$$

where t_0 is the period of the orbit. Substituting $x(t)$ yields

$$\Delta E(x_0) = \omega_0 J_0(KR_g) \cos(Kx_0) \tag{14}$$

with $J_0(z)$ the Bessel function of zero order. For $\frac{2\pi R_g}{a} \gtrsim 1$,one can approximate the Bessel function J_0 by a cosine function as follows

$$J_0\left(\frac{2\pi R_g}{a}\right) \simeq \left(\frac{a}{\pi^2 R_g}\right)^{\frac{1}{2}} \sin\left(\frac{2\pi R_g}{a} - \frac{\pi}{4}\right)$$

with the result

$$\Delta E(x_0) = \omega_0 \left(\frac{a}{\pi^2 R_g}\right)^{\frac{1}{2}} \sin\left(\frac{2\pi R_g}{a} - \frac{\pi}{4}\right), \tag{15}$$

which is the classical expression for the bandwidth. This is the same as obtained in equation (13) in the limit of large n which is to be expected as the large n limit corresponds to classical results.

V. CONCLUSIONS

In this work we have analyzed the electronic spectrum of graphene subjected to a magnetic field perpendicular to the graphene layer and a unidirectional periodic magnetic modulation. We have determined the density of electronic states and the bandwidth of this system. We have also considered the asymptotic expression of bandwidth and its relation to a classical

description. To highlight the effects of modulation on the density of states and bandwidth, we have plotted these quantities as a function of the magnetic field for experimentally relevant parameters. We have found that oscillations in the density of states and the bandwidth are out of phase and larger in amplitude compared to the electrically modulated graphene. We also observe that these oscillations are in phase and smaller in amplitude than those of magnetically modulated standard electron gas system.

VI. ACKNOWLEDGEMENTS

One of us (K.S.) would like to acknowledge the support of the Pakistan Science Foundation (PSF) through project No. C-QU/Phys (129). M. T. would like to acknowledge the support of the Pakistan Higher Education Commission (HEC).

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